Benzoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names: Benzoic acid, 2,3-dihydroxy, tri-TMS
Benzoic acid, 2,3-dihydroxy, TMS
2,3-Dihydroxybenzoic acid, 3tms derivative

Inchi: InChI=1S/C16H30O4Si3/c1-21(2,3)18-14-12-10-11-13(15(14)19-22(4,5)6)16(17)20-23(7,

InchiKey: IPIPJXIWUUYKNS-UHFFFAOYSA-N

Formula: C16H30O4Si3

SMILES: C[Si](C)(C)OC(=O)c1cccc(O[Si](C)(C)C)c1O[Si](C)(C)C

Mol. weight [g/mol]: 370.66

CAS: 3618-19-7

Physical Properties

Property code	Value	Unit	Source
log10ws	1.38		Crippen Method
logp	5.106		Crippen Method
rinpol	1743.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1728.40		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1728.40		NIST Webbook
rinpol	1743.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3618197&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices